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Effects of Thermal-Solutal Convection on Temperature and Solutal Fields under Various Gravitational Orientations

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Introduction

Semiconductor crystals such as $Hg_{1-x}Cd_xTe$ grown by unidirectional solidification Bridgmann method have shown compositional segregations in both the axial and radial directions (Lehoczky et. al..1980, 1981, 1983). Due to the wide separation between the liquidus and the solidus of its pseudobinary phase diagram (Lehoczky and Szofran 1981), there is a diffusion layer of higher HgTe content built up in the melt near the melt-solid interface which gives a solute concentration gradient in the axial direction. The value of effective diffusion coefficient calculated from fitting of the data to 1D model varies with $Hg_{1-x}Cd_xTe$ growth conditions (Szofran 1984).This indicates that the growth condition of the $Hg_{1-x}Cd_xTe$ is not purely diffusion controlled. Because of the higher thermal conductivity in the melt than that in the crystal in the growth system, there is a thermal leakage through the fused silica crucible wall near the melt-solid interface. This gives a thermal gradient in the radial direction. Hart (1971), Thorpe, Hutt and Soulsby (1969) have shown that under such condition a fluid will become convectively unstable as a result of different diffusivities of temperature and solute. It is quite important to understand the effects of this thermosolute convection on the compositional segregation in both axial and radial directions in the unidirectionally solidified crystals under various gravitational directions. To reach this goal, we start with a simplified problem to study the effects of thermal-solutal convection on the temperature and solutal fields under various gravitational orientations. We begin by reviewing model governing equations.

Governing Equations

In this study we adopt the Boussinesq approximation; The equation of state takes the form that density is constant except that in the presence of the gravitational field a buoyancy force exists due to density variations which is caused by the temperature variation and concentration variation in the melt.

Under the Boussinesq approximation and axial symmetric boundary conditions, the governing equations in cylindrical coordinates for incompressible fluid flow of the system are:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + \omega\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial r} + \upsilon\left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial z^2} - \frac{u}{r^2}\right) \quad [1]$$

$$\frac{\partial \omega}{\partial t} + u\frac{\partial \omega}{\partial r} + \omega\frac{\partial \omega}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \upsilon\left(\frac{\partial^2 \omega}{\partial r^2} + \frac{1}{r}\frac{\partial \omega}{\partial r} + \frac{\partial^2 \omega}{\partial z^2}\right) + g(\beta_T(T - T_0) + \beta_C(C - C_0)), \quad [2]$$

$$\frac{u}{r} + \frac{\partial u}{\partial r} + \frac{\partial \omega}{\partial z} = 0 \quad [3]$$

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial r} + \omega\frac{\partial T}{\partial z} = +\alpha_T\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right), \text{ and} \qquad [4]$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial r} + \omega\frac{\partial C}{\partial z} = \alpha_C\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2}\right) \qquad [5]$$

Scale the dimensional variable

The equations can be nondimensionalized by scaling the variables by a factor F; i. e $V = F V^*$. Scaling length by R_C, velocity by ν/R_C, time by R_c^2/ν, pressure by $\rho g \beta_T \Delta T R$, nondimensionalize temperature by setting $\Theta = \frac{T - T_m}{T_m}$ and nondimensionalize solute concentration by setting $\Phi = \frac{C - C_0}{C_0}$. After the scaling and dropping all the *, the dimensionless equations become:

$$\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + \omega\frac{\partial u}{\partial z}\right) = -\frac{\partial p}{\partial r} + \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial z^2} - \frac{u}{r^2}\right), \qquad [6]$$

$$\left(\frac{\partial \omega}{\partial t} + u\frac{\partial \omega}{\partial r} + \omega\frac{\partial \omega}{\partial z}\right) = -\frac{\partial p}{\partial z} + \left(\frac{\partial^2 \omega}{\partial r^2} + \frac{1}{r}\frac{\partial \omega}{\partial r} + \frac{\partial^2 \omega}{\partial z^2}\right)$$

$$+ Gr_T^{1/2}\left(T + (Gr_C/Gr_T)\,C\right), \qquad [7]$$

$$P_r\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial r} + \omega\frac{\partial T}{\partial z}\right) = K\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right); \text{ and } \quad K = \frac{K_i}{K_s};\ i = \text{melt},\ s = \text{solid} \qquad [8]$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial r} + \omega\frac{\partial C}{\partial z} = \frac{1}{S_c}\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2}\right) \qquad [9]$$

Where the thermal and solutal Grashof numbers respectively, Gr_T, Gr_C are defined by:

$$Gr_T = \frac{g\beta_T \Delta T R^3}{\upsilon^2} \quad \text{and} \quad Gr_C = \frac{g\beta_C \Delta C R^3}{\upsilon^2} \qquad [10]$$

The Prandtl number, Pr, and Schmidt number, Sc, are defined by:

$$S_C = \upsilon/\alpha_C \quad \text{and} \quad P_r = \upsilon/\alpha_T. \qquad [11]$$

Compare the nondimensionalized equations with the FIDAP equations, we use the following inputs to the FIDAP for strongly coupled equations

Quantity	Setting		Values used
Density	1		1
Viscosity	1		1
Specific Heat, C_p	P_r	$P_r = \nu / \alpha$	0.233
Conductivity	K_l / K_s or 1		2
Capacity, C_{ps}	1		1
Diffusivity, D	$1/S_c$	$S_c = \nu / D$	0.0143
Thermal Volume Expansion, β_T	G_{rT}	$G_{rT} = g\beta_T \Delta T\, R_c^3 / \nu^2$	
Solutal Volume Expansion, β_s	G_{rs}	$G_{rs} = g\beta_s \Delta C\, R_c^3 / \nu^2$	

These governing equations show that the flow characteristic are determined uniquely by Gr_T, Gr_C, Pr and Sc. These equations have been solved by the FIDAP program developed by Fluid Dynamics International, Inc.The boundary conditions on the velocity field are no slip at all walls. The boundary conditions on the solute field are constant at the top of the melt and satisfy segregation condition at the growth interface.

Conclusions

Preliminary simulation results for the input values listed above and $Gr_C=0$ with $Gr_T=0$ reveal that CdTe compositional profile under 1D diffusion controlled growth condition agree well with the result obtained by Han et. al. (Han et. al. 1992).Fixed grid simulation for $Gr_C=0$ with $Gr_T = 10^4$ has also been obtained.Results indicated that CdTe concentration profiles has been effected by convection due to horizontal thermal gradients.(Figs 2). Although a great effort has been applied, the steady state simulations for the effects of concentration profiles under deformed grids has never been converged. The planed studies will be continued by doing transient simulations.

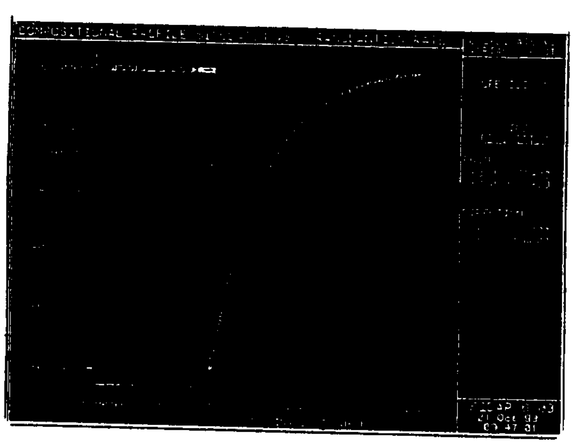

Fig.1. $Gr_C=0$, $Gr_T=0$.

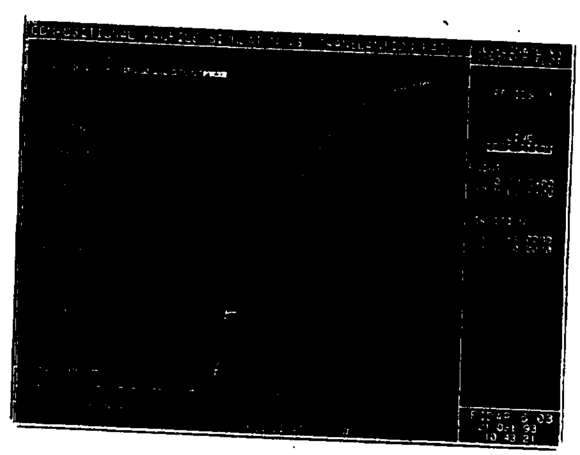

Fig.2 $Gr_C=0$, $Gr_T=10^4$

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